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Monte Carlo simulation of X-ray imaging and spectroscopy experiments using quadric geometry and variance reduction techniques☆

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ABSTRACT

The simulation of X-ray imaging experiments is often performed using deterministic codes, which can be relatively fast and easy to use. However, such codes are generally not suitable for the simulation of even slightly more complex experimental conditions, involving, for instance, first-order or higher-order scattering, X-ray fluorescence emissions, or more complex geometries, particularly for experiments that combine spatial resolution with spectral information. In such cases, simulations are often performed using codes based on the Monte Carlo method. In a simple Monte Carlo approach, the interaction position of an X-ray photon and the state of the photon after an interaction are obtained simply according to the theoretical probability distributions. This approach may be quite inefficient because the final channels of interest may include only a limited region of space or photons produced by a rare interaction, e.g., fluorescent emission from elements with very low concentrations. In the field of X-ray fluorescence spectroscopy, this problem has been solved by combining the Monte Carlo method with variance reduction techniques, which can reduce the computation time by several orders of magnitude. In this work, we present a C++ code for the general simulation of X-ray imaging and spectroscopy experiments, based on the application of the Monte Carlo method in combination with variance reduction techniques, with a description of sample geometry based on quadric surfaces. We describe the benefits of the object-oriented approach in terms of code maintenance, the flexibility of the program for the simulation of different experimental conditions and the possibility of easily adding new modules. Sample applications in the fields of X-ray imaging and X-ray spectroscopy are discussed.

Program summary

Program title: XRMC
Catalogue identifier: AERO_v1_0
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AERO_v1_0.html
Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland
Licensing provisions: GNU General Public License version 3
No. of lines in distributed program, including test data, etc.: 83617
No. of bytes in distributed program, including test data, etc.: 1038160
Distribution format: tar.gz
Programming language: C++.
Computer: Tested on several PCs and on Mac.

☆ This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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Operating system: Linux, Mac OS X, Windows (native and cygwin).

RAM: It is dependent on the input data but usually between 1 and 10 MB.

Classification: 2.5, 21.1.

External routines: XrayLib (https://github.com/tschoonj/xraylib/wiki)

Nature of problem:
Simulation of a wide range of X-ray imaging and spectroscopy experiments using different types of sources and detectors.

Solution method:
XRMC is a versatile program that is useful for the simulation of a wide range of X-ray imaging and spectroscopy experiments. It enables the simulation of monochromatic and polychromatic X-ray sources, with unpolarised or partially/completely polarised radiation. Single-element detectors as well as two-dimensional pixel detectors can be used in the simulations, with several acquisition options. In the current version of the program, the sample is modelled by combining convex three-dimensional objects demarcated by quadric surfaces, such as planes, ellipsoids and cylinders. The Monte Carlo approach makes XRMC able to accurately simulate X-ray photon transport and interactions with matter up to any order of interaction. The differential cross-sections and all other quantities related to the interaction processes (photoelectric absorption, fluorescence emission, elastic and inelastic scattering) are computed using the xraylib software library, which is currently the most complete and up-to-date software library for X-ray parameters. The use of variance reduction techniques makes XRMC able to reduce the simulation time by several orders of magnitude compared to other general-purpose Monte Carlo simulation programs.

Running time:
It is dependent on the complexity of the simulation. For the examples distributed with the code, it ranges from less than 1 s to a few minutes.

1. Introduction

Variance reduction techniques for the simulation of X-ray photon transport allow for the combination of the speed of deterministic methods and the ability of the Monte Carlo approach to simulate photon histories up to the first or higher interaction order under complex experimental conditions. Such techniques have been widely used in the field of X-ray fluorescence spectroscopy [1–5].

Some general-purpose Monte Carlo simulation codes make limited use of variance reduction techniques [6,7], for instance by providing the option of forcing a particle to end its trajectory in a specific region of space. However, most X-ray imaging and spectroscopy applications require a greater computational effort. Expert users often incorporate other types of variance reduction techniques by modifying specific parts of general-purpose Monte Carlo codes. Therefore, the derivation and implementation of such techniques are often considered an art by Monte Carlo software developers.

Bottigli et al. [8] presented a code for the simulation of X-ray imaging and spectroscopy experiments performed on samples described in a three-dimensional regular grid, with elemental composition and mass density specified for each grid node (voxel). In this work, we present a program for the simulation of X-ray imaging and spectroscopy experiments based on the Monte Carlo method by exploiting variance reduction techniques, with a description of the sample geometry based on quadric surfaces. Past versions of this program have been used in medical imaging [9–13], archaeometry [14–16] and beam characterisation [17–19] with X-ray tubes as well as with less conventional X-ray sources (e.g., inverse Compton scattering sources [9–13,17,18]) for planning experimental setups, optimising experimental parameters and comparing theoretical models with experimental results. The code is written entirely in the C++ programming language. A description of the main variance reduction techniques used for the Monte Carlo simulation of X-ray photon transport can be found in Ref. [1–5,8]. The present work instead focuses on a description of the advantages of an object-oriented approach for the general simulation of X-ray imaging and spectroscopy experiments and on the use of quadric surfaces for the geometrical modelling of experiments. The following sections describe the main classes used in the code with their member variables and functions.

2. Method

The standard experimental setup simulated by XRMC consists of an X-ray source, a sample and a detector.

The source can be a point-like source or it can have a three-dimensional Gaussian distribution. The radiation emitted by the source can be unpolarised, partially polarised or fully polarised. The energy spectrum can include a continuous component and a set of discrete energy lines, which can either be monochromatic or follow Gaussian distributions with specified standard deviations.

The sample is composed of a number of materials, called *phases*, which are characterised by their mass density and by their elemental composition, i.e., the atomic numbers and weight fractions of the atomic species that define them. Each phase is assumed to be homogeneous. The sample geometry is specified using a set of three-dimensional objects delimited by quadric surfaces.

The detector can be either a pixel array or a single-element detector. Each pixel/element can have a rectangular or an elliptical shape. It can either record the number of X-ray photons collected by each pixel over a specified exposure time, the total deposited energy of these photons or the full spectrum of the radiation detected by each pixel. The source, the sample and the detector can be placed at arbitrary positions in arbitrary orientations.

XRMC can simulate the history of individual X-ray photons, starting from the source and ending at the detector. The trajectory of a photon is modelled as consisting of a sequence of straight paths, each of which is terminated by an interaction of the photon with a sample atom. The interaction processes that can be simulated by XRMC are the photoelectric effect (eventually followed by fluorescence emission), Rayleigh (elastic) scattering and Compton (inelastic) scattering. The (differential) cross-sections for these interactions and the fluorescence line energies are computed